

# SENSITIVITY STUDIES FOR METHANE AND CARBON MONOXIDE RETRIEVALS FROM SENTINEL-5 PRECURSOR

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## ABSTRACT

Carbon monoxide (CO) has a large impact on air quality and methane (CH<sub>4</sub>) is an important anthropogenic greenhouse gas. Detailed and continuous observations of these gases are necessary to better assess their impact on climate and atmospheric pollution. Abundances of both gases can be obtained from ESA's future satellite mission Sentinel-5 Precursor (S-5P).

This work shows first results from the verification activities undertaken at the University of Bremen. For this, the BESD (Bremen Optimal Estimation DOAS) retrieval algorithm is used that has already been successfully applied to CO<sub>2</sub> retrieval from SCIAMACHY satellite data.

First simulations show that the adaption of BESD to the S-5P specifications results in reasonable results, which will lead to a detailed comparison of BESD results with the operational retrieval algorithms for CO and CH<sub>4</sub>. This will contribute to achieving high quality results for the final data product of CO and CH<sub>4</sub> from the S-5P satellite mission.

Key words: Methane, carbon monoxide, Sentinel-5 Precursor.

## 1. INTRODUCTION

Methane (CH<sub>4</sub>) is after carbon dioxide the most important anthropogenic greenhouse gas. To better assess the impact on the climate system a close monitoring of CH<sub>4</sub> emissions is necessary. While there are airborne instruments available that are able to accurately monitor emissions on local scales [1], global coverage can only be achieved using satellite instruments. After the decommissioning of SCIAMACHY [2, 3] onboard ENVISAT, GOSAT [4, 5] is the only remaining satellite in orbit measuring CH<sub>4</sub> with sensitivities down to the surface where most sources and sinks are located. While GOSAT has a very high horizontal resolution of about 10 km it is lacking complete coverage due to gaps of about 260 km between individual measurements [6]. The

next upcoming satellite mission providing global coverage of measurements of CH<sub>4</sub> sensitive down to the lowest atmospheric layers is ESA's Sentinel-5 Precursor (S-5P) mission scheduled for launch in 2015. S-5P is a single instrument mission with the absorption spectrometer TROPOMI (TROPOspheric Monitoring Instrument) measuring in the ultraviolet (UV), the visible (VIS), the near-infrared (NIR) and the shortwave infrared (SWIR) spectral range. With a swath of 2600 km and a horizontal nadir resolution of 7 km × 7 km in the SWIR band where CH<sub>4</sub> is measured TROPOMI has daily global coverage [7]. The SWIR channel of TROPOMI was designed to retrieve carbon monoxide (CO) which is an important atmospheric pollutant impacting air quality. The retrieval of precise and accurate CH<sub>4</sub> information from this band is more challenging.

In this contribution first results from the scientific verification activities for the total CO column and for the column averaged dry air mole fractions XCH<sub>4</sub> will be presented. Using the BESD (Bremen Optimal Estimation DOAS) retrieval algorithm that is successfully applied also to XCO<sub>2</sub> retrieval from SCIAMACHY data [8, 9], sensitivity studies on simulated observations will be shown taking into account various atmospheric scenarios with varying parameters, for example, for clouds, solar zenith angle and surface spectral reflectance.

## 2. TROPOMI ON SENTINEL-5 PRECURSOR

The absorption spectrometer TROPOMI is a passive optical instrument relying on backscattered solar radiation. It is planned for launch in 2015 into a sun synchronous orbit with a local time of about 13:35 h. The instrument covers four wavelength ranges in the UV from 270–320 nm, in the UV/VIS from 310–500 nm, in the NIR from 675–775 nm and in the SWIR from 2305–2385 nm. It thereby can monitor a wide range of important atmospheric constituents including ozone, NO<sub>2</sub>, SO<sub>2</sub>, CO, CH<sub>4</sub>, CH<sub>2</sub>O and aerosol properties [7]. This work concentrates on absorption bands in the NIR and SWIR to retrieve information on CH<sub>4</sub> and CO. The spectral resolution in the NIR and SWIR is about 0.38 nm and 0.25 nm respectively. Due to its wide swath of about 2600 km in across track

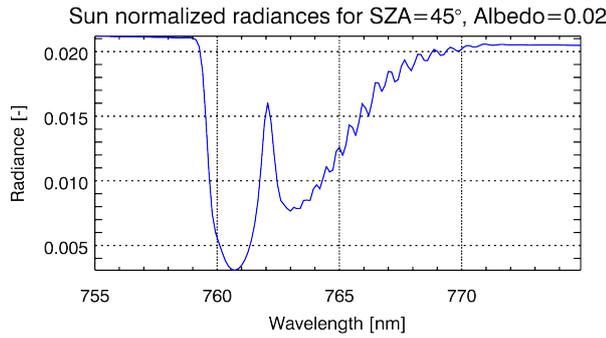


Figure 1. Simulated oxygen A band absorption in the NIR part of the observed electromagnetic spectrum using the SCIATRAN radiative transfer model for an albedo of 0.02 and a solar zenith angle of 45°.

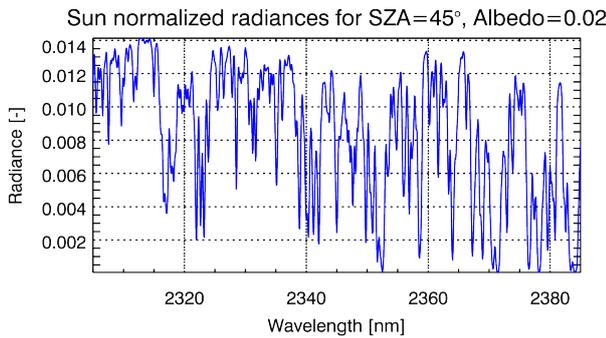


Figure 2. As Figure 3 but for the SWIR wavelength range.

direction with individual ground scenes of  $7 \text{ km} \times 7 \text{ km}$  (at nadir), TROPOMI reaches global coverage in one day.

### 3. RELEVANT ABSORPTION BANDS

Relevant for the work presented here are the absorption bands in the NIR and SWIR part of the observed electromagnetic spectrum. Fig. 1 shows a simulated spectrum in the NIR band exhibiting strong absorption lines due to the Oxygen A-band absorption. The simulation has been performed using the SCIATRAN radiative transfer model [10].

In the SWIR band, absorption lines of  $\text{CH}_4$ ,  $\text{CO}$  and  $\text{H}_2\text{O}$  interfere resulting in a complicated absorption spectrum that is shown in Fig. 2. Absorption of the individual gases in this band is shown in Fig. 3. Note that the  $\text{CO}$  absorption lines are more than an order of magnitude less intense than the  $\text{CH}_4$  and water vapour absorption in the same wavelength region.

### 4. BESD RETRIEVAL ALGORITHM

The Bremen Optimal Estimation DOAS (BESD) retrieval algorithm [8, 9] relies on fitting various parameters in-

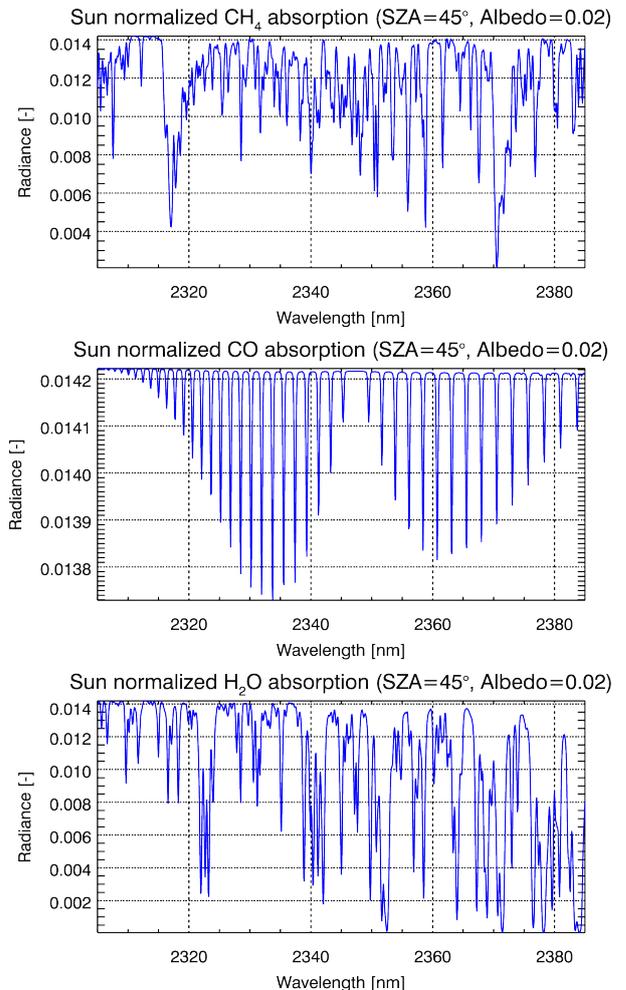


Figure 3. Single gas absorption in the SWIR part of the observed electromagnetic channels for an albedo of 0.02 and a solar zenith angle of 45°. The figure shows absorptions of methane (top), carbon monoxide (centre) and water vapour (bottom).

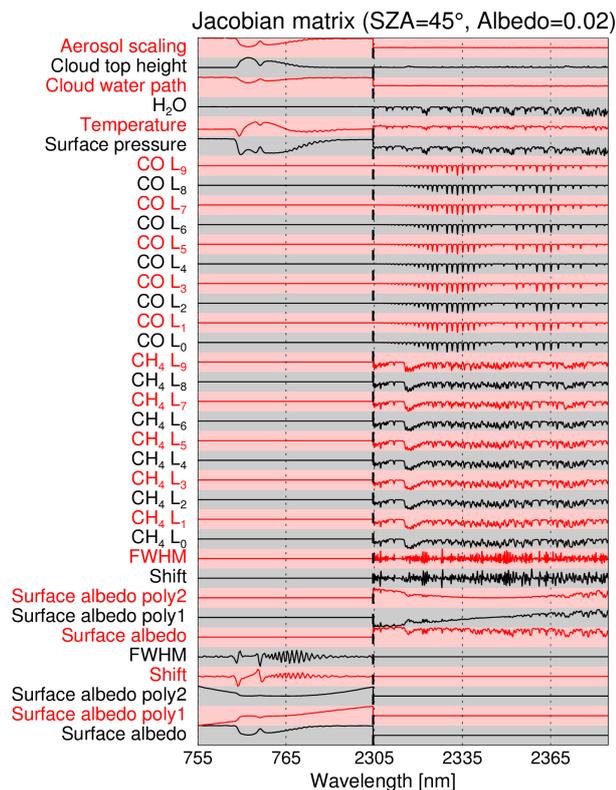


Figure 4. Example of the Jacobians of all retrieval parameters used for the BESD-TROPOMI retrieval algorithm.

cluding cloud top height and cloud water path in two fit windows in the NIR and SWIR spectral range. In case of TROPOMI, the retrieval uses the absorption bands described in Section 3, i.e. the 1.6  $\mu\text{m}$  band used for SCIAMACHY is replaced by the 2.3  $\mu\text{m}$  band. By merging the two spectral windows, scattering parameters can be effectively distinguished from the trace gas absorptions in the SWIR window [8]. Using an optimal estimation approach weakly constrained by adequate a priori knowledge, the retrieval iteratively fits a forward model spectrum to the measured (or simulated) data using the Jacobians (or weighting functions) with respect to the fit parameters simultaneously for both fit windows. The algorithm is described in detail in [8] at the example of  $\text{CO}_2$  retrieval from SCIAMACHY. The forward model of each iteration including the Jacobians is computed using the SCIATRAN radiative transfer model [10].

Fig. 4 shows exemplarily for a surface spectral albedo of 0.02 and a solar zenith angle of  $45^\circ$  the Jacobians of the parameters used for the  $\text{CO}$  and  $\text{CH}_4$  retrieval from simulated TROPOMI measurements. The radiative transfer model SCIATRAN is also used to compute the simulated spectrum.

A typical fit result for the NIR and SWIR fit window is shown in Fig. 5 and Fig. 6, respectively. The synthetic retrieval is based on simulated measurements using a surface albedo of 0.2 and a solar zenith angle of  $45^\circ$ . In this

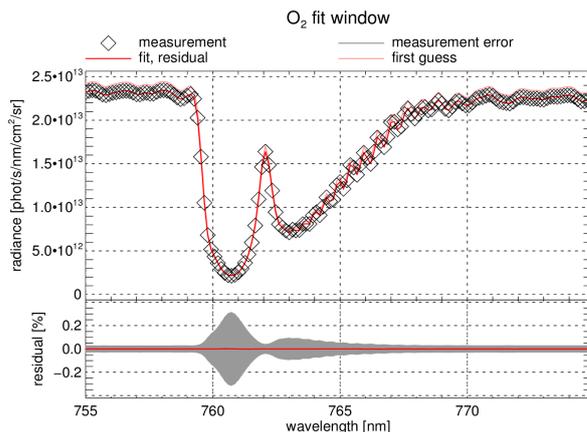


Figure 5. Retrieval result for the NIR fit window using simulated spectra for a surface albedo of 0.2 and a solar zenith angle of  $45^\circ$ . The upper panel shows the measured (simulated) radiance in black diamonds and the fit in red. The pale red line shows the first guess for the retrieval which is not identical to the simulated radiance due to the choice of different parameters used to generate the simulated data. The bottom panel shows the fit residual in red and the measurement error based on the signal to noise ratio indicated by the grey shaded area.

case the simulated data did not include a cloud, while the retrieval's first guess assumed a cloud of 500 m geometrical thickness consisting of fractal ice crystals with 50  $\mu\text{m}$  effective radius, a cloud top height of 10 km and an optical thickness of about 0.3 (at 500 nm).

## 5. FIRST SENSITIVITY STUDIES ON SYNTHETIC DATA

The BESD retrieval algorithm was used to determine the retrieval noise and bias as a function of a range of param-

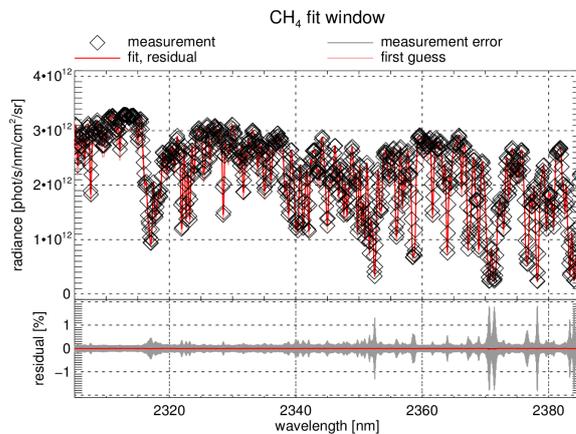


Figure 6. As Figure 5 but for the SWIR fit window.

eters. For this, the parameters for the simulated spectra were modified while the retrieval algorithm had constant a priori and first guess information. Fig. 7 shows the retrieval noise based on a reference signal to noise ratio of 100 in the continuum for a dark scene (albedo of 0.05) and low sun (solar zenith angle of  $70^\circ$ ). This corresponds to the threshold requirement. For bright scenes, the signal to noise ratio is accordingly higher.

The influence of the wavelength dependence of the surface albedo cannot be completely accounted for by a second order polynomial as used in the retrieval. The induced bias for different albedo scenarios is shown in Fig. 8. In case of CO, the retrieval bias is generally below 2% except for extreme solar zenith angles over snow which result also in a very low signal to noise ratio. In case of CH<sub>4</sub>, the bias is below 0.25% except for high solar zenith angles over snow and water which generally have a very low albedo in the SWIR spectral range. The spectral albedo scenarios are based on the ASTER Spectral Library through the courtesy of the Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California (©1999, California Institute of Technology) and the Digital Spectral Library 06 of the US Geological Survey in the same manner as used by [8].

Clouds generally can have a strong impact on trace gas retrievals. This is somewhat mitigated due to the explicit accounting of scattering in the retrieval algorithm. Fig. 9 shows the introduced retrieval bias based on a simulated cloud at 10 km altitude applying a surface albedo of 0.1 and different solar zenith angles for varying cloud optical thickness of 0.01, 0.1 and 1.0. For CO the error is below about 0.4% and for CH<sub>4</sub> below about 0.25%.

Additionally to the cloud optical thickness also the cloud top height was varied from 6 km to 21 km for different solar zenith angles (see Fig. 10). In this case, high solar zenith angles in combination with low clouds can lead to a large bias. Generally, however, the introduced retrieval bias is below 0.25% for CO and below 0.05% for CH<sub>4</sub> with an exception for a very low cloud.

In general, an effective cloud mask filtering for TROPOMI can prevent large errors due to clouds.

## 6. CONCLUSIONS

A number of synthetic retrievals have been performed on simulated data to assess the performance of the BESD algorithm applied to TROPOMI spectral data. Tested scenarios included variations in spectral albedo, cloud optical thickness and cloud top height.

For CO, the retrieval bias for the tested scenarios are well below the 8% threshold requirement. The CO single measurement precision is generally well below 8% as well. Only for very low albedos in combination with high solar zenith angles, the precision can be deteriorated. For CH<sub>4</sub> precision and bias are generally well below 1% which is

in line with the requirements for CH<sub>4</sub> for the S-5P mission. The next step in the verification process is to extend the number of scenarios tested and compare the results with the operational prototype algorithms for CH<sub>4</sub> and CO.

## ACKNOWLEDGEMENTS

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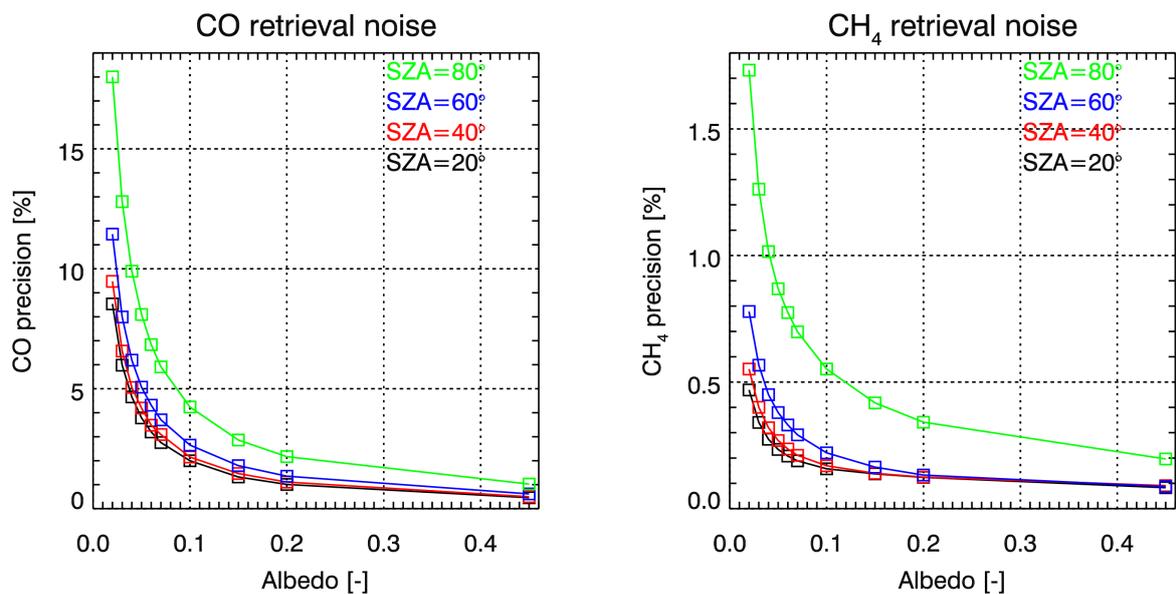


Figure 7. Retrieval noise depending on the surface albedo and solar zenith angle (different colours) for CO (left panel) and CH<sub>4</sub> (right panel).

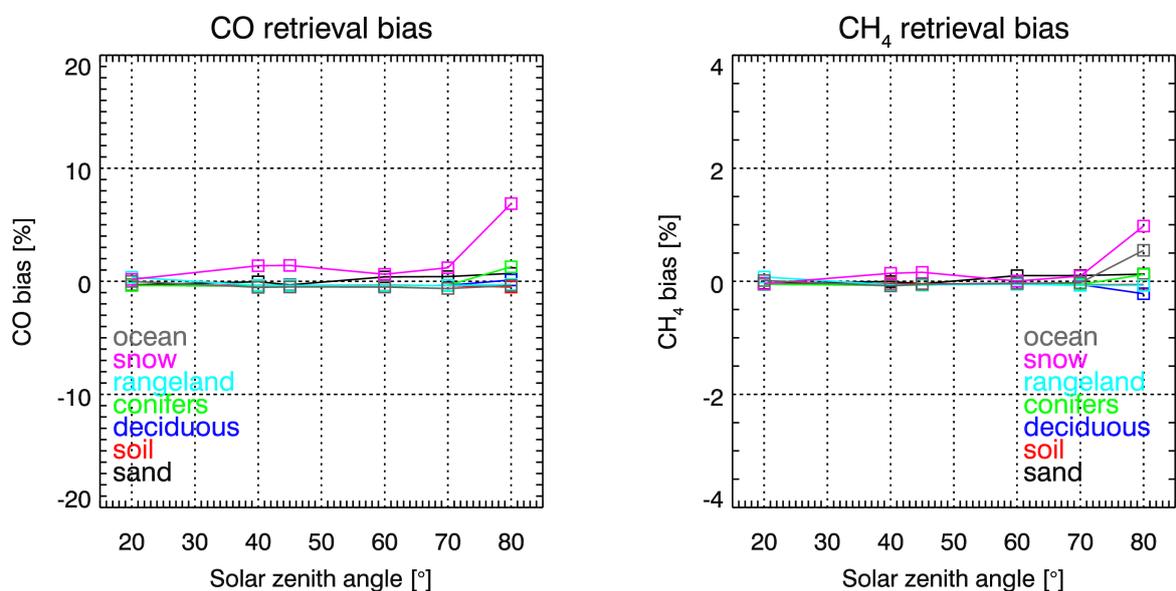


Figure 8. Retrieval bias based on different solar zenith angles and spectral albedo scenarios (different colours) for CO (left panel) and CH<sub>4</sub> (right panel).

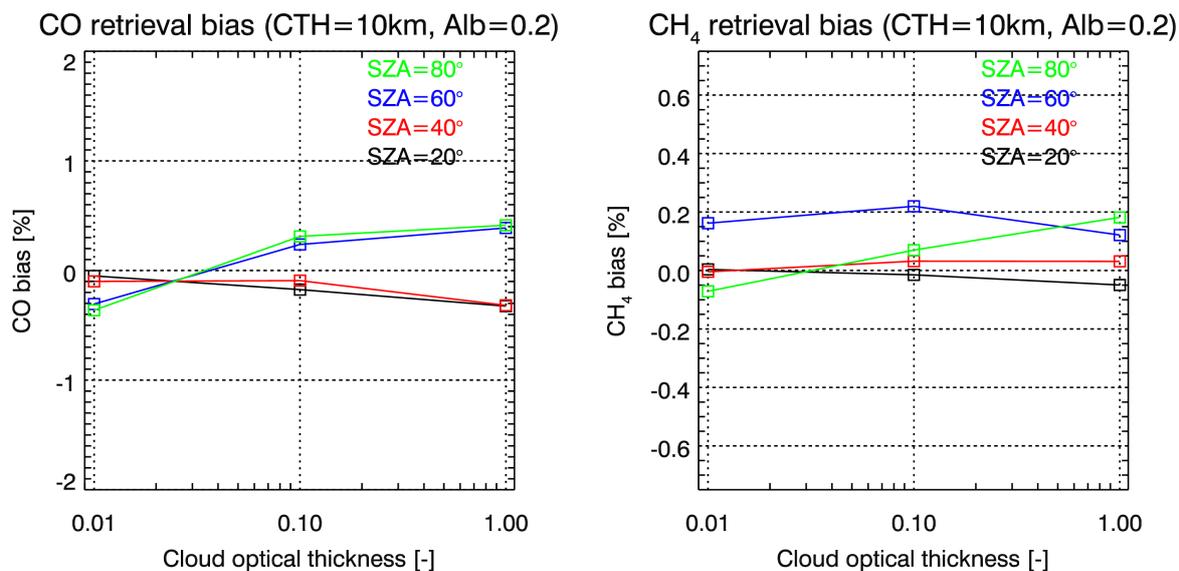


Figure 9. Retrieval bias based on varying cloud optical thickness and different solar zenith angles (different colours) for CO (left panel) and CH<sub>4</sub> (right panel). The scenarios have been computed using a surface albedo of 0.2 and a cloud top height of 10 km.

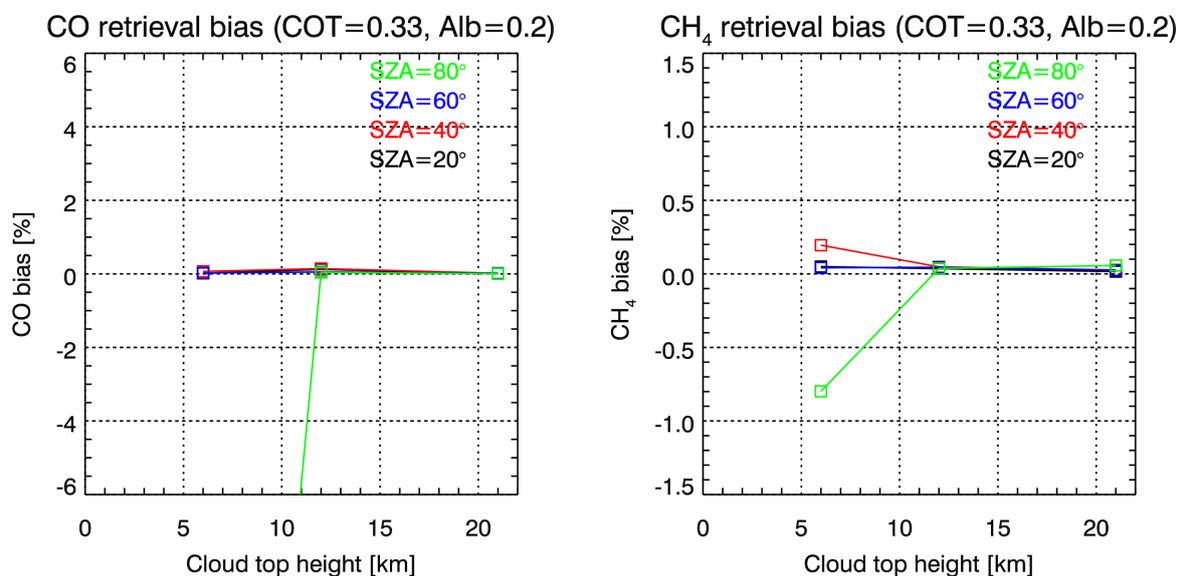


Figure 10. Retrieval bias based on varying cloud top height and different solar zenith angles (different colours) for CO (left panel) and CH<sub>4</sub> (right panel). For all scenarios the cloud optical thickness was constant at 0.33 and the surface albedo was 0.2.

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